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Preserving algebraic invariants with Runge–Kutta methods

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Abstract

We study Runge–Kutta methods for the integration of ordinary differential equations and the retention of algebraic invariants. As a general rule, we derive two conditions for the retention of such invariants. The first is a condition on the coefficients of the methods, the second is a pair of partial differential equations that otherwise must be obeyed by the invariant. This paper extends previous work on multistep methods in Iserles (Technical Report NA1997/13, DAMTP, University of Cambridge, 1997). The cases related to the retention of quadratic and cubic invariants, perhaps of greatest relevance in applications, are thoroughly discussed. We conclude recommending a generalized class of Runge–Kutta schemes, namely Lie-group-type Runge–Kutta methods. These are schemes for the solution of ODEs on Lie groups but can be employed, together with group actions, to preserve a larger class of algebraic invariants without restrictions on the coefficients. © 2000 Elsevier Science B.V. All rights reserved.

1. Background and notation

In this paper we study the numerical solution by Runge–Kutta methods of the ordinary differential system

$$\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y}), \quad \boldsymbol{y}(0) = \boldsymbol{y}_0 \tag{1}$$

for $t \geqslant 0$, where $\boldsymbol{y} \in \mathbb{R}^d$ and $\boldsymbol{f} : \mathbb{R}^+ \times \mathbb{R}^d \to \mathbb{R}^d$ is a Lipschitz function. We assume that the exact solution $\boldsymbol{y}(t)$ of (1) is known to obey the condition that there exists a nontrivial function $\rho : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ (or a family of such functions) such that

$$\rho(\boldsymbol{y}(t), \boldsymbol{y}_0) \equiv 0, \quad t \geqslant 0. \tag{2}$$

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We say, in this case, that the solution $\boldsymbol{y}$ is *ρ-invariant.* [1] Sometimes, we say that ρ is a first integral of (1) or that it is a conservation law or that it defines a manifold $\mathscr{M}$ on which the solution $\boldsymbol{y}$ evolves. All these terms will be used interchangeably in the course of the paper. The degree of smoothness of ρ is related to the degree of smoothness of the function $\boldsymbol{f}$ defining the differential equation (1). Moreover, we say that ρ is a *strong invariant* if there exists a nonempty open set $\mathscr{U}$ in $\mathbb{R}^d$ such that for all $\boldsymbol{y}_0 \in \mathscr{U}$ the solution y with initial value $y(0) = y_0$ satisfies $\rho(\boldsymbol{y}(t), \boldsymbol{y}_0) \equiv 0$ for $t \geqslant 0$. In the present paper, we restrict our attention to the case when ρ is a strong invariant.

There exist numerous problems in applied mathematics that can be paraphrased in the above formalism. Just to mention a few, many physical systems evolve in time and yet their total energy or the phase-space volume or angular momentum stay put. In particular, the Hamiltonian energy of *Hamiltonian systems* is preserved. See [11,26,27,19] for further examples and applications.

Given the differential equation (1) in tandem with the invariance condition (2) and having introduced a subdivision $t_0 = 0 < t_1 < \cdots < t_n < \cdots$ of the integration interval, we say that a one-step numerical method

$$\boldsymbol{y}_{n+1} = \boldsymbol{\phi}_h(\boldsymbol{y}_n), \quad h = t_{n+1} - t_n \tag{3}$$

is *ρ-invariant* (or equivalently *$\mathscr{M}$-invariant*) if

$$\rho(\boldsymbol{y}_n, \boldsymbol{y}_0) = 0, \quad \forall n \geqslant 0 \tag{4}$$

for all $h < \bar{h}$, or, equivalently,

$$\boldsymbol{y}_0 \in \mathscr{M} \Rightarrow \boldsymbol{y}_n \in \mathscr{M} \quad \text{for all } n \geqslant 0, \tag{5}$$

$\mathscr{M}$ being the manifold defined by the function ρ [7].

Conditions that ensure preservation of invariants by Runge–Kutta methods have been already considered in a number of papers. Let us mention first the work of Cooper [4] who proved that there exists a subclass of Runge–Kutta methods that preserve quadratic invariants: all the functions ρ of the form $\rho(\boldsymbol{y}, \boldsymbol{y}_0) = \sum_{i,j=1}^{d} \alpha_{i,j} y^i y^j + \sum_{i=1}^{d} \beta_i y^i + \gamma$ where $\alpha_{i,j}, \beta_i$ and γ are coefficients allowed to depend on y_0. The very same schemes that preserve quadratic invariants preserve also canonical symplectic structure, a result independently discovered in [26]. Later, in their investigation on numerical methods and isospectral flows, Calvo et al. proved that there is no subclass of such schemes that preserves also cubic laws: in other words, given an RK method that preserves quadratic manifolds, it is always possible to construct a differential equation with a cubic invariant ρ for which (4) does not hold for $n = 1, 2, \ldots$ (see [3,27]).

With regard to other classes of methods and their preservation of conservation laws, we mention that results along similar lines have been derived by Iserles for *multistep methods* and for *Taylor-type* methods [14] and independently by Hairer and Leone in the context of symplecticity [10]. We will follow here the approach of [3,27,14] and show that cubic invariance is equivalent to requiring a very strong condition on the invariant, namely that it has to be the solution of a partial differential equation called the Bateman equation. Although the Bateman-equation condition arises also in the case of multistep and Taylor-type methods [14], Runge–Kutta methods are a case apart since their error term is not a constant times a derivative of the function but is a linear combination

[1] Note that in this paper we discuss algebraic invariance. Therefore, ρ should be confused with neither a symmetry nor a differential invariant. We refer the reader to [15] and to the references therein for a treatment of symmetry invariants and to [2] for discussion of differential invariants.

of mixtures of derivatives of various orders (elementary differentials [12]), a feature that makes RK schemes different from many other numerical schemes for integration of ODEs.

The paper is organised as follows. In Section 2 we discuss classical RK methods and their condition for invariance, deriving the Bateman equation (a second-order partial differential equation), and a third-order partial differential equation, for the algebraic invariant ρ. The main result of the paper is presented in Section 3. First, we analyse the third-order counterpart of the Bateman equation. Secondly, we focus on the case of polynomial conservation laws and deduce that Runge–Kutta schemes cannot preserve any polynomial conservation law except for linear and quadratic.

We conclude with Section 4, relating Runge–Kutta methods with a larger class of numerical scheme on Lie groups of which classical RK schemes are but one representative. Numerical methods that stay on Lie groups are nowadays a very active area of research, and constitute an alternative approach to more classical stabilization and projection techniques, and differential-algebraic equations.

Although the material of Section 4 is not original, it furnishes an important example how to bypass the restrictions of this paper and of [14], which limit the applicablity of classical time-stepping methods when the retention of algebraic invariants is at issue. The material of Section 4 is relevant not just because Lie groups represent a major instance of invariants and symmetries, with a wide range of applications, but also for a deeper reason. Traditionally, numerical analysis of differential equations concerned itself mainly with methods that minimise error and cost. Lately, greater attention is being paid to correct modelling of geometric features of differential equations: invariants, asymptotics, symmetries etc. The main thrust of [14] and of this paper is that little can be expected of classical methods insofar as invariants are concerned. The lesson of Section 4 and of much of contemporary effort in geometric integration is that a very powerful approach toward correct rendition of invariants originates in the introduction of ideas from differential geometry and topology to numerical mathematics [2]. We firmly believe that this will increasingly become a major area of computational activity.

2. Necessary condition for invariance: the Bateman equation and its third-order counterpart

Without loss of generality, let us assume that the differential equation (1) is *autonomous*, namely that the function $\boldsymbol{f} \equiv \boldsymbol{f}(\boldsymbol{y})$ does not depend explicitly on time. Throughout the exposition, we also assume that $\boldsymbol{f}$ and ρ are analytic functions.

The exact solution of (1) is approximated numerically by means of a v-stage Runge–Kutta method,

$$\begin{aligned} \boldsymbol{Y}_i &= \boldsymbol{y}_n + h\sum_{j=1}^{v} a_{i,j}\boldsymbol{K}_j, \\ \boldsymbol{K}_i &= \boldsymbol{f}(\boldsymbol{Y}_i), \quad i = 1,2,\ldots,v, \\ \boldsymbol{y}_{n+1} &= \boldsymbol{y}_n + h\sum_{i=1}^{v} b_i\boldsymbol{K}_i, \end{aligned} \tag{6}$$

defined in terms of the *RK matrix* $A = (a_{i,k})$ and the *RK weights* $\boldsymbol{b} = (b_i)$ [12,13].

Recall that any system (1) that is ρ-invariant and autonomous can be written in the *skew-gradient* form

$$\boldsymbol{y}' = S(\boldsymbol{y})\nabla\rho(\boldsymbol{y}), \tag{7}$$

whereby $S(\cdot)$ is a $d\times d$ skew-symmetric matrix [18,25], and in particular we will restrict our attention to the case of two variables, i.e. $d=2$, whereby (7) yields

$$\begin{aligned} y_1' &= \psi(\boldsymbol{y})\frac{\partial\rho(\boldsymbol{y})}{\partial y_2},\\ y_2' &= -\psi(\boldsymbol{y})\frac{\partial\rho(\boldsymbol{y})}{\partial y_1} \end{aligned} \tag{8}$$

for some arbitrary smooth function $\psi:\mathbb{R}^2\to\mathbb{R}$. Since we wish to derive necessary conditions for invariance, we may assume without loss of of generality that $\psi\equiv 1$.

Proposition 1. *Assume that the function $\rho\in C^2[\mathbb{R}^2]$ is not a solution of the* Bateman equation

$$\mathscr{B}(u) = \left(\frac{\partial u}{\partial y_2}\right)^2\frac{\partial^2 u}{\partial y_1^2} - 2\frac{\partial u}{\partial y_1}\frac{\partial u}{\partial y_2}\frac{\partial^2 u}{\partial y_1\partial y_2} + \left(\frac{\partial u}{\partial y_1}\right)^2\frac{\partial^2 u}{\partial y_2^2} = 0 \tag{9}$$

[5], *where $u\equiv u(y_1,y_2)$. A necessary condition for the RK method* (6) *to preserve ρ for all $h<\bar{h}$ is*

$$b_i a_{i,j} + b_j a_{j,i} = b_i b_j, \quad i,j = 1,2,\ldots,v. \tag{10}$$

Proof. For clarity's sake we suppress the dependence of ρ on the initial condition $\boldsymbol{y}_0$. Expanding in powers of h and using (6), we have

$$\begin{aligned} \rho(\boldsymbol{y}_{n+1}) &= \rho\left(\boldsymbol{y}_n + h\sum_{i=1}^{v} b_i\boldsymbol{K}_i\right)\\ &= \rho(\boldsymbol{y}_n) + \sum_{k=1}^{\infty}\frac{h^k}{k!}\sum_{i_1,\ldots,i_k=1}^{v} b_{i_1}\cdots b_{i_k}\\ &\quad\times\sum_{l=1}^{k}\binom{k}{l}\frac{\partial^k\rho(\boldsymbol{y}_n)}{\partial^{k-l}y_1\partial^l y_2}f_1(\boldsymbol{Y}_{i_1})\cdots f_1(\boldsymbol{Y}_{i_{k-l}})f_2(\boldsymbol{Y}_{i_{k-l+1}})\cdots f_2(\boldsymbol{Y}_{i_k}), \end{aligned} \tag{11}$$

whereby the index of $\boldsymbol{f}$ denotes either its first or its second component, namely,

$$f_1(\boldsymbol{Y}_i) = \frac{\partial\rho(\boldsymbol{Y}_i)}{\partial y_2}, \quad f_2(\boldsymbol{Y}_i) = -\frac{\partial\rho(\boldsymbol{Y}_i)}{\partial y_1}, \quad i = 1,2,\ldots,v.$$

Let us assume that $\rho(\boldsymbol{y}_n)=0$ and let us focus on the terms up to order 2 in h. Using the identity

$$\boldsymbol{y}_n = \boldsymbol{Y}_i - h\sum_{j=1}^{v} a_{i,j}\boldsymbol{K}_j,$$

and expanding the functions $\partial\rho/\partial y_l$, $l=1,2$, we obtain

$$\frac{\partial\rho}{\partial y_1}(\boldsymbol{y}_n)\frac{\partial\rho}{\partial y_2}(\boldsymbol{Y}_i)-\frac{\partial\rho}{\partial y_2}(\boldsymbol{y}_n)\frac{\partial\rho}{\partial y_1}(\boldsymbol{Y}_i)$$

$$=-h\sum_{j=1}^{v}a_{i,j}\left[\frac{\partial^2\rho(\boldsymbol{Y}_i)}{\partial y_1^2}\frac{\partial\rho(\boldsymbol{Y}_i)}{\partial y_2}\frac{\partial\rho(\boldsymbol{Y}_j)}{\partial y_2}-\frac{\partial^2\rho(\boldsymbol{Y}_i)}{\partial y_1\partial y_2}\frac{\partial\rho(\boldsymbol{Y}_i)}{\partial y_2}\frac{\partial\rho(\boldsymbol{Y}_j)}{\partial y_1}\right.$$

$$\left.-\frac{\partial^2\rho(\boldsymbol{Y}_i)}{\partial y_1\partial y_2}\frac{\partial\rho(\boldsymbol{Y}_i)}{\partial y_1}\frac{\partial\rho(\boldsymbol{Y}_j)}{\partial y_2}+\frac{\partial^2\rho(\boldsymbol{Y}_i)}{\partial y_2^2}\frac{\partial\rho(\boldsymbol{Y}_i)}{\partial y_1}\frac{\partial\rho(\boldsymbol{Y}_j)}{\partial y_1}\right].$$

Taking into account that $\boldsymbol{Y}_j=\boldsymbol{Y}_i+\mathcal{O}(h)$, we expand the above expression at $\boldsymbol{Y}_i$ to obtain

$$\frac{\partial\rho}{\partial y_1}(\boldsymbol{y}_n)\frac{\partial\rho}{\partial y_2}(\boldsymbol{Y}_i)-\frac{\partial\rho}{\partial y_2}(\boldsymbol{y}_n)\frac{\partial\rho}{\partial y_1}(\boldsymbol{Y}_i)=-h\sum_{j=1}^{v}a_{i,j}\mathscr{B}(\rho)(\boldsymbol{Y}_i)+\mathcal{O}(h^3).$$

By the same token,

$$\frac{h^2}{2}\sum_{i,j=1}^{v}b_ib_j\sum_{l=1}^{2}\binom{2}{l}\frac{\partial^2\rho(\boldsymbol{y}_n)}{\partial^{2-l}y_1\partial^l y_2}f_1(\boldsymbol{Y}_{i_1})\cdots f_1(\boldsymbol{Y}_{i_{2-l}})f_2(\boldsymbol{Y}_{i_{2-l+1}})\cdots f_2(\boldsymbol{Y}_{i_2})$$

$$=\frac{h^2}{2}\sum_{i,j=1}^{v}b_ib_j\mathscr{B}(\rho)(\boldsymbol{Y}_i)+\mathcal{O}(h^3).$$

Hence, reordering indices, we obtain

$$\rho(\boldsymbol{y}_{n+1})=\frac{1}{2}h^2\sum_{i,j=1}^{v}(b_ib_j-b_ia_{i,j}-b_ja_{j,i})\mathscr{B}(\rho)(\boldsymbol{Y}_i)+\mathcal{O}(h^3).$$

Thus, unless ρ is a solution of the Bateman equation (9), annihilation of the $\mathcal{O}(h^2)$ term requires relations (10). □

The Bateman equation (9) plays a very important role also in the context of linear multistep methods and retention of conservation laws. As a matter of fact, Iserles proves that a necessary condition for ρ-invariance of a multistep method is that ρ obeys the Bateman equation [14].

The following result characterises the level sets of the solutions of the Bateman equation (9): essentially, they are determined by linear functions!

Proposition 2 (Iserles [14]). *Solutions $\rho(x,y)$ of the Bateman equation* (9) *such that $\rho(x,y)=\text{const}$ have the form*

$$\rho(x,y)=\omega(\alpha x+\beta y+\gamma),$$

where α,β and γ are arbitrary constants and $\omega\equiv\omega(z)$ is an arbitrary analytic function.

An important consequence of the above result is that linear multistep methods (and in general Taylor-type methods) can be invariant solely in linear manifolds.

We have seen that

$$\rho(\boldsymbol{y}_{n+1}) = \frac{1}{2}h^2 \sum_{i,j=1}^{v} (b_i b_j - b_i a_{i,j} - b_j a_{j,i}) \mathscr{B}(\rho)(\boldsymbol{Y}_i) + \mathcal{O}(h^3),$$

whereby the $\mathcal{O}(h^3)$ term contains partial derivatives of ρ of order greater than two. Hence, if ρ is a quadratic manifold, all these derivatives are zero and we are left with the condition

$$\rho(\boldsymbol{y}_{n+1}) = \frac{1}{2}h^2 \sum_{i,j=1}^{v} (b_i b_j - b_i a_{i,j} - b_j a_{j,i}) \mathscr{B}(\rho)(\boldsymbol{Y}_i),$$

which implies that condition (10) is necessary and sufficient for the retention of quadratic conservation laws, a result well known and understood in the literature of Runge–Kutta methods [4,3,27].

Theorem 3. *A necessary condition for preserving a nonquadratic algebraic invariant ρ is that $\rho \in C^3[\mathbb{R}]$ is a solution of the partial differential equation*

$$\mathscr{L}(u) = \left(\frac{\partial u}{\partial y_2}\right)^3 \frac{\partial^3 u}{\partial y_1^3} - 3\left(\frac{\partial u}{\partial y_2}\right)^2 \frac{\partial u}{\partial y_1} \frac{\partial^3 u}{\partial y_1^2 \partial y_2}$$
$$+ 3\frac{\partial u}{\partial y_2}\left(\frac{\partial u}{\partial y_1}\right)^2 \frac{\partial^3 u}{\partial y_1 \partial y_2^2} - \left(\frac{\partial u}{\partial y_1}\right)^3 \frac{\partial^3 u}{\partial y_2^3} = 0. \quad (12)$$

Proof. Proceeding as in Proposition 1 but carrying the expansions a step further, we obtain, as a first contribution, the term

$$\frac{1}{3}h^3 \sum_{i,j,l=1}^{v} b_i b_j b_l \mathscr{L}(\rho)(\boldsymbol{Y}_i) + \mathcal{O}(h^4)$$

when $k=3$ in (11). The second contribution is obtained from the term for $k=2$ in (11): substituting $\boldsymbol{y}_n = \boldsymbol{Y}_i - h\sum_{l=1}^{v} a_{i,l}\boldsymbol{K}_l$ and collecting similar terms, we obtain

$$\frac{1}{2}h^2 \sum_{i,j=1}^{v} b_i b_j \left[\frac{\partial^2 \rho(\boldsymbol{y}_n)}{\partial y_1^2} f_1^2 + 2\frac{\partial^2 \rho(\boldsymbol{y}_n)}{\partial y_1 \partial y_2} f_1 f_2 + \frac{\partial^2 \rho(\boldsymbol{y}_n)}{\partial y_2^2} f_2^2\right]$$
$$= \frac{1}{2}h^2 \sum_{i,j=1}^{v} b_i b_j \mathscr{B}(\rho)(\boldsymbol{Y}_i) - \frac{1}{2}h^3 \sum_{i,j,l=1}^{v} b_i b_j a_{i,l} \mathscr{L}(\rho)(\boldsymbol{Y}_i) + \mathcal{O}(h^4),$$

whereby $f_1 \equiv f_1(\boldsymbol{Y}_i)$ and $f_2 \equiv f_2(\boldsymbol{Y}_i)$. Finally, the last contribution arises from the series expansion of the $\mathcal{O}(h)$ term. We have

$$\frac{\partial \rho}{\partial y_1}(\boldsymbol{y}_n)\frac{\partial \rho}{\partial y_2}(\boldsymbol{Y}_i) - \frac{\partial \rho}{\partial y_2}(\boldsymbol{y}_n)\frac{\partial \rho}{\partial y_1}(\boldsymbol{Y}_i)$$
$$= \frac{\partial \rho(\boldsymbol{Y}_i)}{\partial y_2}\left\{\frac{\partial \rho(\boldsymbol{Y}_i)}{\partial y_1} - h\sum_{j=1}^{v} a_{i,j}[\rho_{y_1 y_1}(\boldsymbol{Y}_i) f_1(\boldsymbol{Y}_j) + \rho_{y_1 y_2}(\boldsymbol{Y}_i) f_2(\boldsymbol{Y}_j)]\right.$$

$$+\frac{1}{2}h^2\sum_{j,l=1}^{v} a_{i,j}a_{i,l}[\rho_{y_1y_1y_1}(\boldsymbol{Y}_i)f_1(\boldsymbol{Y}_j)f_1(\boldsymbol{Y}_l)+2\rho_{y_1y_1y_2}f_1(\boldsymbol{Y}_j)f_2(\boldsymbol{Y}_2)+\rho_{y_1y_2y_2}f_2(\boldsymbol{Y}_j)f_2(\boldsymbol{Y}_l)]\Bigg\}$$

$$+\frac{\partial\rho(\boldsymbol{Y}_i)}{\partial y_1}\Bigg\{\frac{\partial\rho(\boldsymbol{Y}_i)}{\partial y_2}-h\sum_{j=1}^{v} a_{i,j}[\rho_{y_1y_2}(\boldsymbol{Y}_i)f_1(\boldsymbol{Y}_j)+\rho_{y_2y_2}(\boldsymbol{Y}_i)f_2(\boldsymbol{Y}_j)]$$

$$+\frac{1}{2}h^2\sum_{j,l=1}^{v} a_{i,j}a_{i,l}[\rho_{y_1y_1y_2}(\boldsymbol{Y}_i)f_1^2(\boldsymbol{Y}_j)+2\rho_{y_1y_2y_2}f_1(\boldsymbol{Y}_j)f_2(\boldsymbol{Y}_j)+\rho_{y_2y_2y_2}f_2^2(\boldsymbol{Y}_j)]\Bigg\}+\mathcal{O}(h^3).$$

Let us focus on the term

$$\sum_{i,j=1}^{v} b_i a_{i,j}\rho_{y_2}(\boldsymbol{Y}_i)\rho_{y_1y_1}(\boldsymbol{Y}_i)f_1(\boldsymbol{Y}_j)$$

and similar expressions. We write this term in the form

$$\frac{1}{2}\sum_{i,j=1}^{v} b_i a_{i,j}\rho_{y_2}(\boldsymbol{Y}_i)\rho_{y_1y_1}(\boldsymbol{Y}_i)f_1(\boldsymbol{Y}_j)+\frac{1}{2}\sum_{i,j=1}^{v} b_j a_{j,i}\rho_{y_2}(\boldsymbol{Y}_j)\rho_{y_1y_1}(\boldsymbol{Y}_j)f_1(\boldsymbol{Y}_i)$$

and expand in series whilst exploiting the relation

$$\boldsymbol{Y}_j=\boldsymbol{Y}_i+h\sum_{l=1}^{v}(a_{j,l}-a_{i,l})\boldsymbol{K}_l.$$

We have

$$\frac{1}{2}\sum_{i,j=1}^{v} b_i a_{i,j}\rho_{y_2}(\boldsymbol{Y}_i)\rho_{y_1y_1}(\boldsymbol{Y}_i)f_1(\boldsymbol{Y}_j)$$

$$=\frac{1}{2}\sum_{i,j=1}^{v} b_i a_{i,j}\rho_{y_2}(\boldsymbol{Y}_i)\rho_{y_1y_1}(\boldsymbol{Y}_i)\rho_{y_2}(\boldsymbol{Y}_i)$$

$$-h\sum_{i,j,l=1}^{v} b_i a_{i,j}(a_{i,l}-a_{j,l})\rho_{y_2}(\boldsymbol{Y}_i)\rho_{y_1y_1}(\boldsymbol{Y}_i)\,[\rho_{y_1y_2}f_1(\boldsymbol{Y}_l)+\rho_{y_2y_2}f_2(\boldsymbol{Y}_l)]+\mathcal{O}(h^2)$$

and

$$\frac{1}{2}\sum_{i,j=1}^{v} b_j a_{j,i}\rho_{y_2}(\boldsymbol{Y}_j)\rho_{y_1y_1}(\boldsymbol{Y}_j)\rho_{y_2}(\boldsymbol{Y}_i)$$

$$=\frac{1}{2}\sum_{i,j=1}^{v} b_j a_{j,i}\rho_{y_2}(\boldsymbol{Y}_i)-h\sum_{l=1}^{v}(a_{j,l}-a_{i,l})(\rho_{y_1y_2}f_1+\rho_{y_2y_2}f_2)\rho_{y_1y_1}(\boldsymbol{Y}_j)\rho_{y_2}(\boldsymbol{Y}_i)$$

$$-\frac{1}{2}h\sum_{i,j,l=1}^{v} b_j a_{j,i}(a_{j,l}-a_{i,l})\rho_{y_2}(\boldsymbol{Y}_i)\,[\rho_{y_1y_1y_1}(\boldsymbol{Y}_i)f_1+\rho_{y_1y_1y_2}(\boldsymbol{Y}_i)f_2]\rho_{y_2}(\boldsymbol{Y}_i)+\mathcal{O}(h^2).$$

Expanding in an identical manner all similar terms, we observe that the terms containing two second derivatives of ρ sum up to zero, hence we are left with terms containing just one second derivative and one third derivative of the function ρ. After some tedious algebra along the lines of [3,27], the contribution of the $k=1$ term in (11) reduces to

$$-\frac{1}{2}h^2\sum_{i,j=1}^{v}(b_i a_{i_j}+b_j a_{j,i})\mathscr{B}(\rho)(\boldsymbol{Y}_i)+\frac{1}{2}h^3\sum_{i,j,l=1}^{v}b_j a_{j,i}a_{i,l}\mathscr{L}(\rho)(\boldsymbol{Y}_i)+\mathcal{O}(h^4).$$

Collecting all the relevant terms, we obtain

$$\rho(\boldsymbol{y}_{n+1})=\frac{1}{2}h^2\sum_{i,j=1}^{v}(b_i b_j-b_i a_{i,j}-b_j a_{j,i})\mathscr{B}(\rho)(\boldsymbol{Y}_i)$$
$$+\frac{1}{6}h^3\sum_{i,j,l=1}^{v}(b_i b_j b_l-3b_i b_j a_{i,l}+3b_i a_{i,j}a_{j,l})\mathscr{L}(\rho)(\boldsymbol{Y}_i)+\mathcal{O}(h^4),$$

where the coefficients of $\mathscr{B}$ and $\mathscr{L}$ are exactly those derived in [3,27], in the context of cubic invariants.

Assume now that ρ does not obey the Bateman equation (see above), whose level sets are straight lines. Hence, in order to annihilate the $\mathcal{O}(h^2)$ term, condition (10) must be satisfied by the coefficients of the RK scheme in question.

In order to annihilate the $\mathcal{O}(h^3)$ term, we have two possibilities: either the coefficients of the scheme obey $\Upsilon=O$, where

$$\begin{aligned}\Upsilon_{i,j,l}=&\,b_i b_j b_l-(b_i b_j a_{i,l}+b_j b_l a_{j,i}+b_l b_i a_{lj})\\&+(b_i a_{i,j}a_{j,l}+b_j a_{j,l}a_{l,i}+b_l a_{l,i}a_{i,j})=0,\quad\forall i,j,l=1,\dots,v\end{aligned}\tag{13}$$

(which has been already encountered in [3,27] in a discussion of cubic invariants) or ρ obeys the differential equation (12). However, it is well known that condition (10) and $\Upsilon=O$ are contradictory [3,27], therefore the only possibility is that the differential condition (12) is satisfied. □

3. On the solutions of the equation $\mathscr{L}(u)=0$

In this section we wish to analyse some properties of the solutions of the partial differential equation (12). Following the same approach as [14], we distinguish two cases. Firstly, we note that when $\partial\rho/\partial y_2$ then ρ does not depend on the second variable, hence the system (8) can be reduced to the univariate case which is trivial to integrate: from $\rho(y_1,y_2)=f(y_1)$, we have

$$y_1'=0,$$
$$y_2'=-f(y_1),$$

hence $y_1=c$ is constant and $y_2=-f(c)t+y_2(0)$.

Let us assume thus that $\partial\rho/\partial y_2\neq 0$ at some point, hence, as a consequence of the analyticity of ρ, the same is true in a proper neighbourhood $\mathscr{U}$. Because of the implicit function theorem, there exists a function η, such that

$$\rho(y_1,y_2)=0\quad\Leftrightarrow\quad y_2=\eta(y_1)\quad\forall\boldsymbol{y}\in\mathscr{U},$$

hence $\rho(y_1, \eta(y_1)) = 0$. To avoid confusion, let us denote such independent variable by x; thus,

$$\rho(x, \eta(x)) = 0. \tag{14}$$

Differentiating $\rho(x, \eta(x)) = 0$ with regards to x, we have

$$\frac{\partial \rho(x, \eta(x))}{\partial y_1} + \frac{\partial \rho(x, \eta(x))}{\partial y_2}\eta'(x) = 0,$$

from which we deduce that

$$\eta' = -\frac{\partial \rho(x, \eta(x))}{\partial y_1}\left[\frac{\partial \rho(x, \eta(x))}{\partial y_2}\right]^{-1}.$$

Further differentiation of (14) implies that

$$\mathscr{B}(\rho)(x, \eta(x)) + \left[\frac{\partial \rho(x, \eta)}{\partial y_2}\right]^3 \eta'' = 0,$$

as in [14]. In particular, we deduce that

$$\eta'' = -\mathscr{B}(\rho)(x, \eta(x))\left[\frac{\partial \rho(x, \eta)}{\partial y_2}\right]^{-3}. \tag{15}$$

Differentiating (14) for a third time, we obtain

$$\mathscr{L}(\rho)(x, \eta) - 3\mathscr{B}(\rho)(x, \eta)\left[\frac{\partial^2 \rho(x, \eta)}{\partial y_1 \partial y_2} + \frac{\partial^2 \rho(x, \eta)}{\partial y_2^2}\eta'\right] + \left[\frac{\partial \rho(x, \eta)}{\partial y_2}\right]^4 \eta''' = 0. \tag{16}$$

Assume that ρ obeys the partial differential equation (12). Substituting in (16) the expression for η'' and dividing by $(\partial\rho/\partial y_2)^2$, which we are assuming not equal identically to zero, we deduce

$$\eta''' \frac{\partial \rho(x, \eta)}{\partial y_2} + 3\eta'' \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial \rho(x, \eta)}{\partial y_2}\right) = 0. \tag{17}$$

Lemma 4. *Assume that* $\partial\rho/\partial y_2 \neq 0$. *Then all solutions of the equation* (17) *obey the differential equation*

$$\mathscr{B}(\rho)(x, \eta(x))) = \text{const.}$$

Proof. We distinguish two cases. Firstly $\eta'' = 0$, in which case the assertion is satisfied because of (15), choosing the constant equal to zero. Otherwise, it is true that $\eta'' \neq 0$ in a certain neighbourhood of x. Hence, we can write

$$\frac{\eta'''}{\eta''} = -3\frac{(\mathrm{d}/\mathrm{d}x)(\partial\rho/\partial y_2)}{\partial\rho/\partial y_2},$$

and, integrating both sides with respect to x, we obtain

$$\log \eta'' = -3 \log \frac{\partial \rho}{\partial y_2} + \text{ an integration constant,}$$

from which we deduce that

$$\eta'' = K\left(\frac{\partial \rho}{\partial y_2}\right)^{-3},$$

K being an arbitrary constant of integration. The result follows by comparing the above expression for η'' with (15). □

Theorem 5. *Assume that $\rho(x,y)$ is a polynomial in x,y of degree $n>2$, that $\rho_y \neq 0$ and that* (1) *has no other conservation laws except for ρ. Then the RK scheme* (6) *cannot preserve ρ for all sufficiently small $h>0$.*

Proof. As a consequence of the above lemma, the problem reduces to studying solutions that render the Bateman operator $\mathscr{B}$ constant. Note that if $\rho(x,y)$ is a polynomial of degree n in x and y, then

$$\rho_{xx}\rho_y^2 - 2\rho_{xy}\rho_x\rho_y + \rho_{yy}\rho_x^2$$

is a polynomial of degree $(n-2)+2(n-1)=3n-4$. In particular, it follows that $3n-4=n$ for $n=2$, while $3n-4>n$ for all $n\geqslant 3$. Assume that

$$\rho(x,y)=ax^2+bxy+cy^2+dx+ey+f=0.$$

Direct computation reveals that

$$\tfrac{1}{2}\mathscr{B}(\rho)=(4ac-b^2)[\rho(x,y)-f]+ae^2-bde+cd^2,$$

hence $\mathscr{B}(\rho)$ is constant, provided that so is ρ. If $n>2$ then $\mathscr{B}(\rho)$ is a proper polynomial in x and y of degree strictly greater then n. Therefore, the system must admit a conservation law other than ρ, of order lower then n if ρ is a factor of the polynomial $\mathscr{B}(\rho)$, larger than n otherwise. This, rules out the important case when ρ is the only integral of the system. □

It has been already established in [3] that Runge–Kutta schemes cannot preserve all arbitrary cubic algebraic invariants. The method of proof in [3] is based on the construction of a specific cubic integral, depending on the coefficients of a scheme which cannot be preserved by the method.

In passing, we mention that, as in the case of Proposition 2, the results of Theorem 5 can be extended to analytic functions of polynomials in the following manner. Assume that ρ is not a polynomial but an analytic function ω of $q(x,y)$, namely $\rho(x,y)=\omega(q(x,y))$. Differentiating and substituting into $\mathscr{B}(\rho)=\text{const}$, we obtain $\omega'(q(x,y))\mathscr{B}(q)=K$, hence, if q is such that $\mathscr{B}(q)=\text{const}$, also $\omega'(q)$ is constant and we obtain a new solution. Thus, the solutions of $\mathscr{B}(\rho)=\text{const}$ are defined up to an arbitrary analytic function ω. This reflects the observation that the manifolds $\{\rho(\boldsymbol{x})=c\}$ and $\{\omega(\rho(\boldsymbol{x}))=\omega(c)\}$ are identical for bijective ω.

Theorem 5 does not rule out the existence of 'proper' sufficiently smooth functions that may be automatically preserved by the Runge–Kutta scheme for sufficiently small h. Seeking an example of such function, we employ the technique of separation of variables. Assume that $\rho(x,y)=v(x)w(y)$, whereby v and w are two C^3 functions of x and y respectively such that $v',w'\neq 0$, hence v and w are at least linear functions. Then the condition $\mathscr{L}(\rho)=0$ is equivalent to

$$\frac{v'''v^2}{v'^3}-3\frac{v''v}{v'^2}+3\frac{w''w}{w'^2}-\frac{w'''w^2}{w'^3}=0$$

(the prime denoting differentiation with respect to the independent variable) which results in an identical ordinary differential equation for the functions v and w, namely

$$\frac{z'''z^2}{z'^3}-3\frac{z''z}{z'^2}=K, \quad z\equiv z(t),$$

where K is an arbitrary constant. When $K=0$, we can reduce the above third-order differential equation into a second-order one by integration,

$$z'' = cz^3,$$

whereby c is an arbitrary integration constant. The solution of the latter is given in implicit form by

$$t = \pm \int_0^{z(t)} \frac{2\mathrm{d}s}{\sqrt{2cs^4 + 4C_1}} + C_2,$$

where c, C_1 and C_2 are arbitrary integration constants. This, however, is unlikely to represent an invariant of practical importance. In general, the determination of all level sets of (12) is incomplete, although we believe that virtually all nonquadratic invariants of interest are excluded and, anyway, it is trivial to check by direct differentiation whether $\mathscr{L}(\rho)=0$ for any specific function ρ.

4. Runge–Kutta methods in a Lie-group formulation

Although we have already seen that the equation $\mathscr{L}(\rho)$ admits solutions that are not necessarily linear or quadratic in y_1, y_2, the sheer complexity of (17) reveals that such manifolds described by $\rho(y_1, y_2)=0$ are exceptional. Moreover, recall that $\mathscr{L}(\rho)=0$ is merely a necessary condition for invariance. We deduce that generic retention of conservation laws by means of classical RK integration cannot be achieved easily, if at all.

A standard way to treat ODEs with invariants that classically are not automatically preserved by RK methods is to reformulate the invariants as constraints and use a differential–algebraic approach [20]. Discussion on numerical preservation of invariants can be traced already to the early 1970s, especially in the fields of constrained mechanics and electronic circuits [6]. There exists a rich literature on Runge–Kutta methods applied to the solution of differential equations with algebraic invariants (DAEs) and these methods, essentially based on projections, have proved themselves to be very effective and successful in many practical applications [12]. It is sometimes argued that numerical schemes that employ projection damage geometric properties of the underlying problem, and this has provided strong motivation to devise numerical schemes that intrinsically retain the underlying invariants. New types of symmetric projections have been recently introduced by Hairer [8] so that not only the invariant, but most of the remaining geometric properties are retained under discretization. Other successful methods for the exact or almost-conservation of invariants are based on splitting of the vector field $\boldsymbol{f}$ into simpler vector fields that are easy to integrate or can be integrated exactly. We refer to the surveys of Hairer [9] and of McLachlan and Quispel [21] for an up-to-date list of techniques for various problems that posses invariants, or, more generally, geometrical structure that one would like to preserve under discretization.

In the last few years there has been a growing interest in devising Lie-group methods that somehow follow the logic of Runge–Kutta schemes in a different manner from the RK schemes for DAEs above. Let us present here the main ideas, referring the reader to [23,17,28] and to the review article [16] for further details.

Lie groups are smooth manifolds endowed with a multiplicative group operation, and without loss of generality, we can identify them with subgroups of $\mathrm{GL}(d,\mathbb{R})$, the set of all $d \times d$ real matrices. (Identical theory can be extended to the complex field.) Familiar examples are $\mathrm{O}(d,\mathbb{R})$, the set of all $d \times d$ orthogonal matrices, and $\mathrm{SL}(d, \mathbb{R})$, the *special linear group* of all $d \times d$ matrices with unit determinant. A (finite-dimensional) Lie algebra is a linear space, closed under commutation. The tangent space at identity of a Lie group is a Lie algebra, hence the importance of the latter construct in any discussion of ODEs evolving on a Lie group. For example, the Lie algebra corresponding to $\mathrm{O}(d, \mathbb{R})$ is $\mathfrak{so}(d, \mathbb{R})$, the linear space of $d \times d$ skew-symmetric matrices, while the Lie algebra of $\mathrm{SL}(d, \mathbb{R})$ is $\mathfrak{sl}(d, \mathbb{R})$, the set of all $d \times d$ matrices with zero trace.

An ordinary differential system on a Lie group G can be always written in the form

$$y' = \gamma(t, y)y, \quad y(0) = y_0,$$

where $y \in G$ and $\gamma : \mathbb{R}^+ \times \mathfrak{g}$, where $\mathfrak{g}$ is the Lie algebra of G, and can be solved so that the numerical approximation resides in G,

$$y_n \in G \quad n = 0, 1, 2, \ldots,$$

provided that $y_0 \in G$, by using a Lie-group modification of classical Runge–Kutta schemes. The main idea is to translate the original ODE in each step from G to $\mathfrak{g}$ by means of the exponential map, $y(t) = \exp(\sigma(t))y_0$, by means of the so-called *dexpinv equation*,

$$\sigma' = \mathrm{dexp}_\sigma^{-1}\gamma, \quad \sigma(t_n) = 0,$$

which acts in $\mathfrak{g}$ instead of G. The function dexp^{-1} is defined as

$$\mathrm{dexp}_\sigma^{-1}(\gamma) = \sum_{k=0}^{\infty} \frac{\mathrm{B}_k}{k!} \mathrm{ad}_\sigma^k \gamma,$$

where the B_k's are Bernoulli numbers [1] and the *adjoint operators* ad^k are k-times iterated commutators of σ with γ, namely $\mathrm{ad}_\sigma^k \gamma = [\sigma, [\sigma, \cdots [\sigma, \gamma] \cdots]]$ (see [23,17,28,16]).

The redeeming feature of this transformation is that $\mathfrak{g}$ is a linear space, while G is usually described by nonlinear conservation laws. Thus, following a construction of Munthe-Kaas [22], an arbitrary Runge–Kutta method can be employed in $\mathfrak{g}$ to produce a numerical approximation $\sigma_{n+1} \approx \sigma(t_{n+1})$, so that

$$y_{n+1} = \exp(\sigma_{n+1})y_n \in G$$

is a numerical approximation for $y(t_{n+1})$ which has the same order as the original RK scheme while remaining in the Lie group. Thus, for example, if $G = \mathrm{SL}(d, \mathbb{R})$, such Lie-group-based RK schemes allow us to preserve to machine accuracy the algebraic invariant $\det y = 1$, a polynomial equation of degree d, while, as we have seen in Section 2, standard RK schemes are bound to fail. Similarly, when $G = \mathrm{O}(d, \mathbb{R})$, with Lie-groups schemes we can use an explicit Lie-group RK method and obtain an orthogonal approximation, while with standard schemes we would require that the RK method obeys condition (10), hence being an implicit scheme.

Such Lie-group schemes do not apply only to Lie groups, but also to a wider class of problems, evolving on *homogeneous spaces* [24], i.e. manifolds on which the dynamics is described by a Lie-group action. (Examples include a d-sphere, a d-torus, isospectral matrices, symmetric matrices, Stiefel and Grassmann manifolds.) In this setting one can obtain the classical Runge–Kutta schemes as a special case of Lie-group Runge–Kutta methods for which the acting group is $\mathbb{R}^d$ with the group operation '$+$' and the manifold acted upon is also $\mathbb{R}^d$. Although such schemes are not yet fully competitive in comparison with the more established DAE methods, a pleasing feature of this approach is that one might choose a different group action to preserve different underlying geometrical features of the problem in question. The search for a good action has to take into account qualitative features that need be preserved, as well as the computational cost of the scheme. This is an area currently under active investigation.

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